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Robust multi-response surface optimization: A posterior preference approach

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Abstract

This paper discusses the use of multi-response surface optimization (MRSO) to select the preferred solutions from among various non-dominated solutions (NDS). Since MSRO often involves conflicting responses, the decision-maker's (DM) preference information should be included in the model in order to choose the preferred solutions. In some approaches this information is added to the model after the problem is solved. In contrast, this paper proposes a three-stage method for solving the problem. In the first stage, a robust approach is used to construct a regression model. In the second phase, non-dominated solutions are generated by the ε-constraint approach. The robust solutions obtained in the third phase are NDS that are more likely to be Pareto solutions during consecutive iterations. A simulation study is then presented to show the effective performance of the proposed approach. Finally, a numerical example from the literature is brought in to demonstrate the efficiency and applicability of the proposed methodology.

1. Introduction

The response surface methodology involves relationships between different variables, such as experimental inputs as controllable factors, and one or more response variables that are uncontrollable, called nuisances (Khuri 1996). The main purpose of this approach is to find the optimum setting of controllable factors, using design and analysis of experiments that will maximize or minimize the responses based on their types. A regression model is applied, considering these factors and responses variables, to illustrate the relationships. Both single responses and multiple responses are common in this approach; to some extent, multiple response surfaces are more suitable for real-world cases, where different responses are considered simultaneously. When several responses are to be analyzed simultaneously, a multi-response optimization problem arises, whose main goal is to find the settings of the input variables that achieve an optimal compromise among the response variables. In this paper, an optimization method is proposed to draw conclusions about the input variables as well as the responses in order to determine the optimum level of each variable. However, as conflicting responses are involved in many cases, a Pareto solution is first extracted from a set of feasible solutions. Then, a decision maker can select the preferred solution based on his/her preferences. In this case, the decision-maker's (DM) preference information is very important to make a reliable decision.

In most multi-response surface optimization (MRSO) methods, the DM's preferences are incorporated using three approaches. The first is the very common approach of prior preference, where it is very difficult to incorporate the DM's preference information precisely, and in many cases, it cannot be determined easily. The second is the progressive approach, which incorporates the DM's preference during the solution procedure. The third one is the posterior preference approach, in which a set of non-dominated solutions (NDS) is presented and the preferred one is selected according to the DM's preference.

Estimating regression models using design and analysis of experiments is the first step in existing approaches. In order to obtain a reliable solution that does not have inordinate effects on the conclusion, these models should not be sensitive to outliers and trends obtained by experiments (Marrona et al. 2006). In other words, models should be as robust as possible to outliers. After designing and performing experiments and finding a robust model, the next step is generally a statistical approach to finally select the controllable factor levels. As the optimization stage is based on the models obtained using regression, estimating a robust regression model is very important that may affect the optimization steps.

A review of the literature reveals that while there are a few papers on the use of posterior approaches in multi-response surface optimization problems, a combination of robust regression and robust response surface methods is new. In other words, this study is the first to use a posterior approach in which the model construction procedure is modified iteratively by robust weighting functions to estimate the regression coefficients with sufficient robustness. Then, a set of robust Pareto (non-dominated) solutions (NDS) is obtained by the ε-constraint method in each iteration. Finally, among these NDS, a novel robust preferred solution is presented that is more likely to be the NDS during consecutive iterations. A novel approach involving two steps, model construction and robust solution selection, is proposed.

Often, it is assumed in linear regression models that residuals are normally distributed. However, sometimes practical applications violate this assumption. The presence of outliers and non-normality of error terms can have a large misleading influence on the performance of classical statistical methods, which are ideal for non-contaminated data under the assumption of normality. A robust approach to statistical modeling and data analysis aims to derive methods that produce reliable parameter estimation in cases where the data follow a given non-normal distribution and there are outliers.

In fact, since the ordinary least squares (OLS) method is very sensitive to outliers, reliable and precise response surface estimates cannot be obtained in the presence of contaminated data. Hence, subsequent calculations in the optimization phase depend on the accuracy of estimated response functions and can be affected by estimation errors that occur in that phase. Moreover, epsilon constraints and robust selection methods improve preferred non-dominated solutions in the selection phase of this type of problem. In this paper, a simulation and a case study are used to show improvement in the final solutions.

The rest of the paper is organized as follows. Section 2 provides a brief review of the relevant literature. Section 3 presents a modified robust model construction procedure. Generating Pareto solutions by the ε-constraint method is presented in Section 4. Section 5 illustrates an application of the proposed methodology. A numerical example is given in Section 6. Finally, Section 7 contains the concluding remarks.

2. Literature review

In industrial cases that require design and analysis of experiments, one issue that often arises is the accuracy of response surfaces obtained by experimental designs. These problems frequently have multiple responses, so it would be interesting to consider outliers and contamination using a robust estimation procedure. There has previously been some research on robust estimation, and multiple responses have also been considered in different ways.

Many authors have investigated multi-response surface optimization problems and proposed different solution approaches (interested readers are referred to Khuri (1996)). These approaches have varied widely, from simple weighted sums (e.g., Antony 2001) to more complex regression and mathematical programming approaches (e.g., Reddy et al. 1997), principal components analysis (e.g., Su and Tong 1997), and dynamic multiple responses (e.g., Tong et al. 2004).

Derringer and Suich (1980) proposed a desirability function approach to MRSO problems, where utility functions are modeled for each response to incorporate the DM's preference into the problems. Pignatiello (1993), Ames et al. (1997), and Ko et al. (2005) presented loss function approaches to incorporate the DM's preference for responses; the first two studies employed a cost matrix to consider process economics and the relative importance of each response. Köksalan and Plante (2003), Xu et al. (2004) and Ames et al. (1997) also employed weight parameters to incorporate DM's preferences.

In all these methods, since the DM's precise preference structure is very important in finding the preferred solution, dual-response surface optimization that incorporates both location and dispersion effects seems a suitable approach. Jeong et al. (2005) suggested a systematic method to determine preference parameter values, such as relative weight values of squared bias and variance in accordance with the DM's preference structure. Although determining preference parameter values compatible with the DM's preference structure is important in MRSO, studies related to this issue have been rare, and most MRSO methods are based on the prior preference approach. Nevertheless, Köksalan and Plante (2003) and Jeong and Kim (2009) suggested that interactive approaches to the solution process be applied until the most preferred solution is obtained.

Some alternative methods, such as least absolute deviations (LAD), robust partial least squares (RPLS), and generalized linear models (GLM), have been used to decrease the effect of outliers. These robust approaches simplify the task of outlier identification by weighting large residuals. Huber (1981) proposed the M-estimator method to obtain robust regression. Morgenthaler et al. (1999) discussed robust response surfaces in chemistry based on experimental design. These authors presented a method in which, although the initial non-robust coefficients are estimated using OLS and the Huber weighting function, the fitted model is modified in some iterations to perform better. Hund et al. (2002) presented methods of outlier detection and evaluated robustness tests using different experimental designs. Bickel and Frühwirthb (2006) compared robust estimators along with their applications. Several authors (e.g., Cummins and Andrews 1995) renamed these estimators as iteratively reweighted least squares (IRLS) because the M- and GM-estimators (which are famous robust estimators in the literature) estimate the coefficients iteratively. Bashiri and Moslemi (2013) proposed an iteratively robust regression procedure based in M-estimators. Considering uncorrelated responses, these authors suggested a simultaneous independent multi-response iterative reweighting (SIMIR) approach. Moslemi et al. (2014) proposed a robust coefficient estimation method assuming correlated responses.

The idea of a posterior preference approach in multiple-objective decision making (MODM) was proposed by Hwang et al. (1979) and Figueria et al. (2005). Lee et al. (2010) proposed a posterior preference approach to dual-response surface optimization. Lee et al. (2011) also presented a posterior preference articulation approach to multi-response surface optimization. The posterior preference approach involves presenting a set of NDS or Pareto solutions where the ε-constraint presented by Haimes et al. (1971) is a common method. The next step after finding the NDS is the selection phase, in which the best solution is obtained among different NDS.

Martin et al. (2005) studied approximating non-dominated sets in continuous multi-objective optimization problems. They noted the lack of a general approach to approximating non-dominated sets in such problems. A continuous approximation to the non-dominated set is obtained by fitting a surface through the points of a discrete approximation, using a local (robust) regression method. The authors provided a general approach that requires only procedures to sample from the set of alternatives and check whether one alternative dominates the others. Then, a discrete approximation of the non-dominated set is needed, which is found by taking a sample and finding the non-dominated subsample. Clyde and Chaloner (1996) surveyed experimental design problems in which utility functions are difficult to assess; they compared designs with respect to several utility functions. Lee et al. (2011) proposed a new interactive selection method to do this. Lee et al. (2012) also proposed an interactive, systematic method to adjust the preference parameters in multi-response surface optimization problems. To obtain a satisfactory compromise, information on decision-maker preferences concerning the trade-offs among the responses should be incorporated into such problems. The preference parameter values are specified in advance or adjusted in an interactive manner. The authors developed an interactive method for MRSO in which the DM provides preference information in the form of pairwise comparisons. The results of these comparisons are used to estimate the preference parameter values.

An analyst generates a solution, and a DM evaluates the solution. Then, the DM adjusts the preference parameter value, based on that evaluation. A new solution is obtained by solving the optimization problem using the adjusted preference parameter values. This process continues until a solution satisfactory to the DM is found. Many existing studies use a similar design, but they propose different preference parameter approaches. Some authors apply the GDF algorithm (Geoffrion et al., 1972) to multi-response problems; values for the marginal rate of substitution between the responses of the current optimal solution are specified by the DM. In Jeong and Kim (2009), the DM adjusts the shape of the desirability function; the bounds or target values of responses are based on the current optimal solution. In another approach, the DM adjusts the preference parameter values indirectly; that is, the DM provides information about preferences, and the analyst bases adjustments to the preference parameter values on that information. Koksalan and Plante (2003) applied a parametric achievement program to MRSO wherein the DM provides a desirable point and the analyst adjusts weight parameters based on the specified desirable point. Lee and Kim (2012) proposed an interactive method based on pairwise comparisons with a dual-response surface methodology. In this study, the minimizing weighted mean squared error (WMSE) is determined by considering squared bias and variance, so an interactive method to consider DM preference information in the form of pairwise comparisons is proposed. Lee and Kim (2013) proposed an empirical study of novel dual-response surface problems based on a posterior approach for multi-response problems. The authors presented a case study in which the target value of after cleaning inspection critical dimension (ACICD) is determined by the dual-response optimization method. The posterior approach to dual-response optimization that they developed was employed to determine the optimal compromise between bias and variability in the electrical characteristics. The use of a posterior preference articulation approach to dual-response surface optimization helped generate a set of potential solutions, allowing the decision maker to select the most preferred solution. They proposed a posterior approach based on the epsilon constraint method and a dual-response surface objective. In the selection phase, they used bias and variability criteria to select the optimum solution.

Some authors have employed various robust methods in multi-response surface optimization problems. Koksoy and Yalcionoz (2006) modeled a problem using mean squared error criteria and utilized a genetic algorithm to solve the model. Koksoy (2008) proposed a nonlinear programming model for robust multi-response problems. Yang and Chou (2005) presented a multi-response simulation-optimization model using a multiple-attribute decision-making method. Kovach and Cho (2008) proposed a new approach to robust design that utilizes D-optimal experimental designs in multi-response optimization problems to overcome the limitations of standard experimental approaches. Baril et al. (2011) first combined a feasibility modeling technique with an interactive multi-objective algorithm to take into account the decision maker's preferences, generating several Pareto-optimal solutions that maintain a probability of constraint satisfaction. Then, they developed a procedure to select a solution from among the reliable Pareto-optimal solutions generated by the algorithm.

Table 1 provides an overview of relevant studies; the bottom row shows the category in which the present study was conducted relative to others. As can be seen, many studies have focused on the optimization phase, where prior multiple-objective decision-making approaches are considered. The most recent research related to this area found in the literature was that conducted by Lee and Kim (2013). Although some posterior approaches have been investigated, and some robust optimization methods have been applied, few papers focus on the robust estimation of response surfaces proposed in the present paper. In addition, novel robust approaches are proposed in the two steps of the posterior multi-response problem, generating non-dominated solutions and selecting a robust solution. Nonetheless, further research that applies the approach proposed in the present paper is required in order to gain more reliable and accurate solutions. Applying this approach is necessary because outliers always exist in experiments, for many reasons, and these data can affect the results. In addition, this paper shows that selecting among solutions that are more robust can result in better solutions.

Insert Table 1 about here

3. Model building and a modified robust method

According to Bashiri and Moslemi (2013), there are two ways to compensate for the effects of outliers: removing the outlier data; or using an inherently robust method. Since detecting outliers is not an easy task and is impractical in many cases, modifying outliers is used in this research.

Let the expected value of the i^{th} response be:

$$E(y_i) = \mu_i(\beta_1, \beta_2, ..., \beta_p) \tag{1}$$

where μ_i is a function defined by unknown coefficients (β_i). For example, if $\mu_i = \beta_1 + \beta_2 x_{1i}$ and x_i are constants, then the estimated expected value of i^{th} response y_i denoted by $\hat{y}_i$ can be obtained by parameter estimates using experimental results.

If the experiments are performed precisely and contain no outliers, then the OLS method provides good estimates of the regression coefficients by minimizing the sum of squared errors (*SSE*) as:

$$SSE = \sum_{i=1}^{n}\left(y_i - \mu_i\left(\hat{\beta}_1, ..., \hat{\beta}_p\right)\right)^2 . \tag{2}$$

However, if the results appear abnormal, which may be a consequence of residual behavior in the experiments (the abnormality occurs when a residual behaves like an outlier), then the coefficients are estimated by minimizing the weighted *SSE* (*WSSE*), as shown in Kutner et al. (2005):

$$WSSE = \sum_{i=1}^{n} w_i\left(y_i - \mu_i\left(\hat{\beta}_1, ..., \hat{\beta}_p\right)\right)^2 . \tag{3}$$

In Equation (3), the weights $w_i^{'}$ s are not pre-assigned because the quality of each y_i is not known in advance. Instead, reasonable weights are determined based on the residuals r_i defined through:

$$r_i = y_i - \mu_i\left(\hat{\beta}_1, ..., \hat{\beta}_p\right) . \tag{4}$$

To make the estimators invariant with respect to the scale of the residuals, $y_i s$ are divided by a scale value that is equal to 1.4826 *MAD*, where *MAD* is the median of the absolute deviations of the residuals from their median and 1.4826 is a bias adjustment for the standard deviation under the normal distribution (Ortiz et al., 2006).

The weights should be inversely proportional to the values of the residuals. In other words, to obtain better estimates of the regression coefficients, larger residuals are weighted less. The Huber weight function given in Equation (5) can be chosen to provide such a weight scheme (Huber, 1981).

$$\begin{cases} w_i = 1 \quad if \quad |r_i| < c \\ w_i = \dfrac{c}{|r_i|} \quad if \quad |r_i| \geq c \end{cases}, \tag{5}$$

where c is a constant determined by the analyst. For 95% efficiency of the regression estimator, c is 1.345.

In short, assuming uncorrelated responses, the modified robust estimation method of a response mean based on Bashiri and Moslemi (2013) is given in Algorithm 1.

1. Divide $y_i s$ by 1.4826 *MAD*
2. Estimate the initial coefficients of the regression model by OLS
3. Calculate the value of residuals and weights using equations (4) and (5)
4. Estimate the new coefficients by minimizing Equation (3)
5. Steps 3 and 4 are repeated iteratively until no significant changes in the estimates are found.

Algorithm 1: The modified model-building algorithm

In order to compare the results obtained, a criterion such as the sum of squared errors (SSE) of estimation is needed. To this aim, the squared error (SE) for each coefficient can be computed based on the pure model in which there is neither contamination nor outliers. Then, for each response surface computed, the squared errors are added together to compute the total SSE. It is clear that the robust regression estimation approach should have less SSE in comparison with the OLS method.

4. Non-dominated solution generation

The ε-constraint approach is one of the most common methods used to generate a set of NDS, where it is assumed that all responses are to be maximized. Since responses are of different types, in order to utilize this approach, all are first transformed into the larger-the-better (LTB) form. This approach consists of solving a set of single-objective problems in which a set of NDS is generated by systematic changes in the ε parameter of the model.

The optimization model for the ε-constraint problem is:

$$\begin{aligned} &\max \hat{y}_j(x) \\ &\text{s.t.} \\ &\hat{y}_i(x) \geq \varepsilon_i \quad ; \quad i = 1,2,3,\ldots,l \ , \ i \neq j \end{aligned} \tag{6}$$

To solve equation (6), one should change the ε-parameters and solve the optimization problems individually. Bounds on each ε_i can be obtained by the DM's preference information, which is presented by utility functions, or by solving each response and finding its optimal value (Lee et al., 2011).

To prevent weak non-dominated solutions, a modified ε-constraint method suggested by Steuer (1986) is proposed:

$$\begin{aligned} &\max \hat{y}_j(x) + \rho \sum_{i=1, i\neq j}^{l} \hat{y}_i(x) \\ &\text{s.t.} \\ &\hat{y}_i(x) \geq \varepsilon_i \quad ; \quad i = 1,2,3,\ldots,l \ , \ i \neq j \ , \end{aligned} \tag{7}$$

where ρ is a small positive constant that prevents from weak non-dominated solutions.

5. The proposed robust method

A robust posterior preference method is proposed to select the best solution among a set of NDS that are generated by the ε-constraint method in each iteration of the response estimation process. Two aspects of robustness are involved: one for estimation of coefficients, and the other for selection of robust non-dominated solutions. The robust non-dominated solutions are those that appear more frequently in the iterative procedure, warranting a more robust posterior preference solution.

The procedure is performed in three steps. The first one is the modified model-building step using the robust weighting method in which regression coefficients are estimated iteratively by Algorithm 1. In the second step, non-dominated solutions for the estimated response functions are generated by changing the ε_i of the ε-constraint method. The third step involves gathering and comparing the NDS that have been generated.

In order to select the preferred robust solution from among the NDS generated in different iterations, the distance between every NDS of the last iteration and the other NDS of previous iterations, called the non-robustness distance (*NRD*), is obtained in the last step using the Mahalanobis distance concept. The Mahalanobis distance in Eq. (8) is a measure of the distance between a point P and a distribution D, where *S* is the covariance matrix. It is a multi-dimensional generalization of the idea of measuring the distance of P from the mean of D in standard deviations,

$$NRD_q = \sqrt{(X_q - \mu_p)^T S^{-1} (X_q - \mu_p)}\ . \tag{8}$$

In Eq. (8), NRD_q is the non-robustness distance obtained for the q^{th} NDS generated in the last iteration, X_q is the vector of the q^{th} NDS control variables generated in the last iteration, and μ_p is the mean vector of control variables. The non-dominated solution with lowest deviation from other previous generated solutions can be selected as the preferred robust non-dominated solution. This measure suggests that the NDS generated in the last iteration with less deviation from others can be considered to be robust.

A novel procedure is proposed here for selecting the solution of a multi-response optimization problem. We do not have the DM's preference about the NDS in our cases, so we propose the confidence level as the statistical point of view based on the Mahalanobis distance. It is clear that the NDS that shows less deviation from all generated solutions may be more robust. This deviation, which is based on statistical computations, can be calculated through the Mahalanobis distance.

As mentioned in Johnson and Wichern (1982), the ellipsoid that is defined by α percent of the observations. This is illustrated in Equation (9) as follows:

$$(X-\overline{X})^T S^{-1}(X-\overline{X}) \leq \chi^2_{p,\alpha} . \qquad (9)$$

In the proposed approach, based on the computed NRD for the NDS in the last iteration, a criterion is assumed and each NDS in the last iteration that is smaller than the proposed square root of the value of the chi-square criterion would be defined as a robust preferred solution. All NDS determined in previous iterations are kept as the coefficients are improved during the robust estimation procedure. Finally, a novel NRD measure is defined to address the possibility that the last sets of NDS are more robust and the selection should only be based on such solutions.

The NRD measures the deviations between the answers of the robust NDS and the other generated NDS. While in a single-response problem the distances of the residuals from the regressed line shows the robustness of the answers, in a multi-response problem the deviations between the robust NDS and the other answers can be considered an index of robustness. In the second phase of the proposed procedure (robust optimization), we assumed that robust NDS are a set of solutions with lowest deviations among other NDS. Since the modified weighting estimation is a converging procedure, the solutions are improved at each step. Hence, the last sets of NDS are more robust. Moreover, the NDS with less deviation from others can be considered a robust set of solutions. Thus, the NRD index acts more like in a situation in which there is no contaminated data. It can be considered a robustness index in this case. The results confirm that the proposed approach can determine more robust NDS. Moreover, the proposed NRD index can be a good measure for evaluation of the robustness of the solutions. Figure 1 illustrates the steps involved in the proposed approach.

Insert Figure 1 about here

To study the proposed robust selection approach, we carried out a simulation with contaminated data. We assumed two responses and the running of twelve experiments. The regression equations consist of two types of coefficients, slope and intercept. Table 2 below shows the design of the hypothetical experiment.

Insert Table 2 about here

For every other experiment, 10% of the data are randomly replaced by contaminated data to study the effect of these outliers on the estimation of the regression coefficients of responses and the NRD index. We generate *m*=500 runs. After applying the robust selection approach to the NRD for each replicate, the NRD index is computed. For each problem, the NDS are generated in two iterations. As y_1 is an objective function, five values for epsilon are suggested for the y_2 utility function. Moreover, the experimental region is $-1 \leq x_i \leq 1$ and the desirable value for y_2 is $90 \leq y_2 \leq 110$, so the values of ε are 0, 5, 10, 15, 20. This simple simulation shows the efficiency of our proposed robust multi-response surface approach. Then the approach is studied in a real-world, complex numerical example.

First we have a case in which two pieces of contaminated data are deleted and the NRD is computed. Then, the proposed approach considering the contaminated data and the classical approach without generating NDS in some iterations are carried out. The results show that the proposed approach has a lower NRD index compared to the classical approach, although the deletion process has the smallest NRD value. The results are shown in Table 3.

Insert Table 3 about here

It is worth mentioning that the NRD criteria in Table 3 is the average of all 500 run problems.

6. Numerical Example

In order to illustrate the application of the proposed methodology and evaluate its performance, the classical tire tread compound problem, originally presented by Derringer and Suich (1980), is used. This problem assumes three chemical materials, silica (x_1), silane (x_2), and sulfur (x_3), and four responses. The decision maker's opinions on each of the four responses are known from the utility functions depicted in Figure 2 (Lee et al. 2011).

Insert Figure 2 about here

A central composite design (CCD) with six center points is applied, where all controllable variables are in the range $-1.633 \le x_i \le 1.633 \;\; ; \;\; i = 1, 2, 3$. The results are shown in Table 4.

Insert Table 4 about here

Based on the above utility functions and experimental results, the upper and the lower bounds of each response, along with the ε-values, can be obtained as follows.

In the first step, a primary quadratic regression model is estimated for each of the four responses:

$$\begin{aligned}
&\hat{y}_1 = 139.12 + 16.4x_1 + 17.88x_2 + 10.91x_3 - 4.01x_1^2 - 3.45x_2^2 - 1.57x_3^2 + \\
&\quad 5.13x_1x_2 + 7.13x_1x_3 + 7.88x_2x_3 \\
&\hat{y}_2 = 1261.11 + 268.15x_1 + 246.50x_2 + 139.48x_3 - 83.55x_1^2 - 124.79x_2^2 - 199.17x_3^2 \\
&\quad + 69.38x_1x_2 + 94.13x_1x_3 + 104.38x_2x_3 \\
&\hat{y}_3 = 400.38 - 99.67x_1 - 31.40x_2 - 73.92x_3 - 7.93x_1^2 - 17.31x_2^2 - 0.43x_3^2 + \\
&\quad 8.75x_1x_2 + 6.25x_1x_3 + 1.25x_2x_3 \\
&\hat{y}_4 = 68.91 - 1.41x_1 + 4.32x_2 + 1.63x_3 + 1.56x_1^2 + 0.06x_2^3 - 0.32x_3^2 - \\
&\quad 1.63x_1x_2 + 0.13x_1x_3 - 0.25x_2x_3
\end{aligned} \tag{10}$$

To generate a set of NDS, the ε-constraint method is employed through

$$\begin{aligned}
&\max \hat{y}_1(x) + \rho\left(\hat{y}_2(x) - \left|\hat{y}_3(x) - 500\right| - \left|\hat{y}_4(x) - 67.5\right|\right) \\
&s.t. \\
&\hat{y}_2(x) \ge 2000 - \varepsilon_2 \\
&\left|\hat{y}_3(x) - 500\right| \le \varepsilon_3 \\
&\left|\hat{y}_4(x) - 67.5\right| \le \varepsilon_4 \\
&x \in \Omega
\end{aligned} \tag{11}$$

Four runs were used to carry out the estimation procedure in the first iteration; the scaled residuals of the four responses are reported in Table 5. Some data seems to be unusual and appears to be contaminated data. The rho value is set as $4{*}10^{-4}$.

Insert Table 5 about here

A set of ε_i for each response is determined to generate a set of non-dominated solutions. The ranges of each ε_i are determined through the upper and lower bounds specified by the decision maker. The minimum and maximum values of ε_i for each response are shown in Figure 2. The increases in the three parameters are then determined, considering the smallest differences in value between the responses. In this case study, four equal-sized intervals are considered to be worth comparing within the ranges for each response. The value of ε_2 ranges from 0 to 1000 with an increment of 250. Similarly, the value of ε_3 ranges from 0 to 100 with an increment of 25 and the value of ε_4 ranges from 0 to 7.5 with an increment of 1.88.

The above optimization formulation is solved 125 (=5*5*5) times, generating 125 solutions; a total of 51 non-dominated solutions remain after infeasible, redundant and dominated solutions are discarded.

The effect of the rho value can be investigated by first generating solutions using the original ε-constraint method. In this case, the first response can be set as the objective function that is to be maximized. The number of epsilon values is set at 5. In the first stage, 51 non-dominated solutions and 51 corresponding sets of ε_i values are obtained. Then, the modified ε-constraint method is employed at several rho values for the 51 sets of epsilon values. We compare the solutions of the modified ε-constraint method with those of the original ε-constraint method. The results are given in Table 6. The first column shows the rho values. The second column shows the number of solutions in which some of the responses improved without deteriorating others, compared with the original ε-constraint method.

Insert Table 6 about here.

In the second step, the robust regression coefficient estimation method is used. For each response, the sum of squares of the residuals is obtained in each iteration. The procedure is repeated until all responses have small-enough changes in coefficient estimation. The final regression model of each response, after four iterations, is given in Table 7.

Insert Table 7 about here

In order to evaluate the performance of the robust regression estimation approach, the sum of squared errors (SSE) of the estimation based on the pure model (the model without any contamination or outliers), the OLS model, and the proposed robust estimation approach in the final iteration should be obtained. The pure model cannot be considered efficient and rational, since in this model outliers and contamination are deleted. In this model, the data that seem to be outliers are first omitted and the pure models are computed, as shown in Table 8.

Insert Table 8 about here

If the pure model is considered to be a reference for future analysis as a good model, one can compare the performance of the proposed robust method and the OLS method based on the pure model, considering the SSE measure. The results of comparison between the proposed robust estimation approach and the OLS method are reported in Table 9.

Insert Table 9 about here

Table 9 clearly shows that the proposed robust estimation approach has a lower SSE in comparison with the OLS method. Thus, one can conclude that the proposed robust estimation approach can be applied instead of the classical OLS method.

It should be noted that at the final stage of model estimation, when the robust estimation approach is applied, the number of generated feasible NDS in the first, second and third iterations are 51, 55 and 47, respectively. Also, the optimization problem in the last iteration is solved 125 times, resulting in 45 groups of acceptable NDS, giving in a grand total of 198 NDS.

The robust preferred solution of the proposed approach is in Table 10. Among all 198 NDS, the preferred robust solutions have smaller non-robustness distances, comparing chi-square criteria with 3 degrees of freedom and α=0.1 equal to 0.584. Consequently, the Mahalanobis distance is the square root of 0.58, which is 0.765. Hence, about 4 out of 45 solutions have smaller Mahalanobis distance values, and the other 41 solutions have greater NRD values. Thus, based on the procedure, they are omitted from the preferred solutions. These solutions are reported in Table 10. The NRD criterion can be helpful in selecting the preferred NDS considering the robustness criterion, and by considering the statistical approach, some of the potentially preferable solutions are selected.

Insert Table 10 about here

A weighted quadratic concave function (Lee et al. 2011) as an overall utility function based on the four individual utility function values is defined by

$$Overal\ Utility\ (U) = 1 - \sum_{i=1}^{4} \lambda_i \left(1 - u_i\right)^2 \ ; \ \lambda = \left(\lambda_1, \lambda_2, \lambda_3, \lambda_4\right) = \left(0.2, 0.2, 0.3, 0.3\right). \tag{12}$$

Since the numerical example in the present study is the same as the one in Lee et al. (2011), the utility function defined in their paper can be helpful in confirming the validity of the proposed method. If the utility function approach is applied to the solutions computed by the proposed robust approach, the results can be helpful in validating that approach. The results are given in Table 11.

Insert Table 11 about here

Considering the proposed procedure in the present study as a novel approach, a statistical-based selection method based on a confidence level is proposed. It is clear that the proposed robust preferred solutions are also sufficiently good solutions, considering the utility function. The proposed robust preferred solutions are as good as the results presented in the literature. Table 11 presents the solutions mentioned in Lee et al (2011), which are obtained through the utility function optimization approach to evaluate the proposed preferred solutions. The results show that the proposed solutions and the NRD criterion can select the solutions as well as the utility function procedure, and that the robustness criterion is well-suited to this approach. Note that the preference of the DM is not needed in the proposed method.

As multi-response surface optimization frequently involves various conflicting responses, in order to obtain a satisfactory settlement, information about the DM's preferences over the tradeoffs among responses should be included in the problem. Most existing MRSO approaches require the DM to state all required preferences completely, which is very difficult in practice. As a remedy to this issue, a posterior preference approach is proposed in MRSO. The proposed method does not require that the preference information be specified in advance. Moreover, a novel approach is applied in the present study, where robustness is employed in the model building stage (response surface estimation). This is a new approach that will absolutely obtain more accurate response surfaces. In addition, a statistical-based selection method based on a confidence level is proposed to provide more robust solutions. This idea is simpler and preferable, since the DM's preference information is not needed in this case.

7. Concluding remarks

A robust multi-response surface optimization methodology based on the posterior preference approach was proposed in the present research. The robustness of the proposed approach is based on two aspects. The first is a focus on robust regression coefficient estimation, and the other one on the efforts to generate more robust non-dominated solutions for multi-response estimated functions. Non-dominated solutions are generated through the ε-constraint method. Using the proposed non-robustness distance measure, the selection phase in the proposed approach is based on the deviation between the robust NDS of the last iteration and those of all previous generated solutions. In this approach, some NDS based on α percentage are selected to be robust preferred solutions. This is a statistical approach to multi-response optimization problems and it leads to a set of preferable NDS. One area for future study would be considering a new robust selection phase based on interactive pairwise methods or employing better estimators. Another approach could be considering correlations between responses.

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Table1. Summary of the literature review

	MRSO				
		MODM Approaches			Robust Multi-Response
Authors	Definition	**Prior**	**Interactive**	**Posterior**	
Khuri (1996)	Multi-response surface methodology	✓	✓		
Antony (2001)	Simple weighted-sum approach	✓			
Su and Tong (2004)	Principal components analysis	✓			
Tong et al. (2004)	Dynamic multiple responses	✓			
Derringer and Suich (1980)	Desirability function approach	✓			
Pignatiello (1993)	Loss function using a cost matrix	✓			
Ames et al. (1997)	Loss function using weight parameters	✓			
Köksalan and Plante (2003) &	Weight parameters		✓		
Xu et al. (2004)	Weight parameters	✓			
Jeong et al. (2005)	Systematic method to determine preference parameter	✓			
Jeong and Kim (2009)	Interactive approach		✓		
Hwang et al. (1979) & Figueria et al. (2005)	Posterior preference approach in MODM			✓	
Lee et al. (2010)	Posterior preference approach to dual response surface optimization			✓	
Lee et al. (2011)	Posterior preference articulation approach			✓	
Lee et al. (2012)	Interactive method to MRSO Based on Pairwise Comparisons		✓		
Lee and Kim (2012)	Interactive Weighting method in DRSO		✓		
Lee and Kim (2013)	Empirical study based on posterior DRSO; Bias and variability criteria for comparison			✓	✓
Koksoy and Yalcionoz (2006), Koksoy (2008), Yang and Chou (2005)	Robust multi-response optimization				✓
Baril et al. (2011)	Interactive multi-objective algorithm		✓		✓
Kovach and Cho (2007)	D-optimal experimental designs in multi-response optimization				✓
Bashiri and Moslemi (2013)	Robust response surface estimation				✓
Moslemi et al. (2014)	Robust correlated response surface estimation				✓
The Proposed Method	**Robust Posterior Multi-response surface method**			✓	✓

Table 2. Experimental data for simulation study

Row	x_1	x_2	y_1	y_2
1	+1	+1	45	101
2	+1	-1	47	102
3	+1	0	48	99
4	0	+1	49	98
5	0	-1	43	96
6	-1	-1	45	103
7	-1	+1	43	102
8	-1	0	42	104
9	0	0	46	101
10	0	0	45	97
11	0	0	45	99
12	0	0	47	95

Table 3. The NRD computed by three approaches

	Proposed approach	**NDS for a data set with deleted outliers**	**OLS and generating one iteration NDS**
Adjusted NRD	1.72	1.45	2.04

Table 4. Experimental data of the tire tread compound problem

Experiment number	x_1	x_2	x_3	y_1	y_2	y_3	y_4
1	-1	-1	+1	102	900	470	67.5
2	+1	-1	-1	120	860	410	65
3	-1	+1	-1	117	800	570	77.5
4	+1	+1	+1	198	2294	240	74.5
5	-1	-1	-1	103	490	640	62.5
6	+1	-1	+1	132	1289	270	67
7	-1	+1	+1	132	1270	410	78
8	+1	+1	-1	139	1090	380	70
9	-1.633	0	0	102	770	590	76
10	+1.633	0	0	154	1690	260	70
11	0	-1.633	0	96	700	520	63
12	0	+1.633	0	163	1540	380	75
13	0	0	-1.633	116	2184	520	65
14	0	0	+1.633	153	1784	290	71
15	0	0	0	133	1300	380	70
16	0	0	0	133	1300	380	68.5
17	0	0	0	140	1145	430	68
18	0	0	0	142	1090	430	68
19	0	0	0	145	1260	390	69
20	0	0	0	142	1344	390	70

Table 5. Scaled residuals of the four responses in the first iteration

Residuals of response 1	Residuals of response 2	Residuals of response 3	Residuals of response 4
1.517707	0.365133	0.954415	0.002499
2.380582	0.726887	0.289316	0.455066
0.292032	0.701443	0.138414	0.793966
0.344831	0.226699	0.032682	1.241554
0.205865	2.219812	0.242829	1.1052
0.165568	0.031065	0.467905	0.68572
1.986447	0.025985	0.051024	0.374079

1.206598	2.618042	0.442152	0.000166
0.014154	0.452444	0.148803	0.222685
0.101901	0.719117	0.006765	0.320732
1.229538	0.477588	2.250479	0.54317
0.82555	0.688186	1.065365	0.691289
0.068577	6.036292	0.023101	0.085831
0.003798	0.876544	0.384379	0.039412
2.059953	0.023761	1.898985	0.658131
2.059953	0.023761	1.898985	0.092879
0.042675	0.212136	**4.008228**	0.458012
0.456538	0.460649	**4.008228**	0.458012
1.90252	0.00202	0.49283	0.004522
0.456538	0.108011	0.49283	0.658131

Table 6. Effect of Rho value in epsilon-constraint methodology

Rho value	Number of solutions which have been improved without any deterioration
10^{-7}	0
10^{-6}	0
10^{-5}	1
10^{-4}	10
$4 * 10^{-4}$	16
$7 * 10^{-4}$	16
10^{-3}	15
10^{-2}	0

Table 7. Final robust regression coefficient estimates of the responses

	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_3$	$\hat{y}_4$
x_1	16.03	297.80	-101.27	-1.28
x_2	15.78	254.50	-31.33	4.17
x_3	12.61	292.40	-72.28	1.76
x_1^2	-4.64	-27.70	11.87	1.52
x_2^2	-2.70	-61.50	5.34	0.15
x_3^2	-2.79	23.70	4.05	-0.35
x_1x_2	10.52	62.00	13.08	-0.83
x_1x_3	2.36	86.10	15.95	-0.62
x_2x_3	2.57	50.30	4.53	0.53
Intercept	140.33	1247.40	391.66	68.81

Table 8. Pure model and OLS coefficient estimates of the responses

	$\hat{y}_1$		$\hat{y}_2$		$\hat{y}_3$		$\hat{y}_4$	
	OLS	Pure	OLS	Pure	OLS	Pure	OLS	Pure
x_1	16.4	16.12	268.15	292.21	-99.67	-102.34	-1.41	-1.21
x_2	17.88	16.1	246.5	253.7	-31.4	-30.2	4.32	4.21
x_3	10.91	12.13	139.48	272.2	-73.92	-72.79	1.63	1.72
x_1^2	-4.01	-4.59	-83.55	-12.32	-7.93	2.57	1.56	1.55
x_2^2	-3.45	-2.6	-124.79	-73.24	-17.31	-1.23	0.06	0.1
x_3^2	-1.57	-2.43	-199.17	12.22	-0.43	3.65	-0.32	-0.34
x_1x_2	5.13	8.98	69.38	64.87	8.75	11.32	1.63	-0.01
x_1x_3	7.13	3.23	94.13	88.21	6.25	10.23	0.13	-0.52
x_2x_3	7.88	4.34	104.38	71.21	1.25	3.45	-0.25	0.23
Intercept	139.12	141.23	1261.11	1252.34	400.38	392.34	68.91	68.85

Table 9. Computed sum of square error (SSE) of the estimated coefficients in OLS and Robust approaches based on pure model

	$\hat{y}_1$		$\hat{y}_2$		$\hat{y}_3$		$\hat{y}_4$	
	Robust	OLS	Robust	OLS	Robust	OLS	Robust	OLS
x_1	0.0081	0.0784	31.2481	578.8836	1.1449	7.1289	0.0049	0.04
x_2	0.1024	3.1684	0.64	51.84	1.2769	1.44	0.0016	0.0121
x_3	0.2304	1.4884	408.04	17614.6	0.2601	1.2769	0.0016	0.0081
x_1^2	0.0025	0.3364	236.5444	5073.713	86.49	110.25	0.0009	0.0001
x_2^2	0.01	0.7225	137.8276	2657.403	43.1649	258.5664	0.0025	0.0016
x_3^2	0.1296	0.7396	131.7904	44685.73	0.16	16.6464	1E-04	0.0004
x_1x_2	2.3716	14.8225	8.2369	20.3401	3.0976	6.6049	0.6724	2.6896
x_1x_3	0.7569	15.21	4.4521	35.0464	32.7184	15.8404	0.01	0.4225
x_2x_3	3.1329	12.5316	437.2281	1100.249	1.1664	4.84	0.09	0.2304
Intercept	0.81	4.4521	24.4036	76.9129	0.4624	64.6416	0.0016	0.0036
SUM	**7.5544**	**53.5499**	**1420.411**	**71894.72**	**169.9416**	**487.2355**	**0.7856**	**3.4084**

Table 10. Final preferred solutions of the proposed methods

Method	$(x_1, x_2, x_3, y_1, y_2, y_3, y_4)$	*Overal Utility*	*NRD*
Proposed Robust Solutions	(-0.01,0.39,-1.1,128.18,1379.12,473.09,68.55)	0.789	0.653
	(0.08,0.5,-1.15,128.87,1411.17,465.71,68.75)	0.787	0.687
	(0.055,0.39,-1.25,126.14,1433.74,477.53,68.07)	0.792	0.69
	(0.012,0.45,-1.1,128.8,1385,469.73,68.78)	0.788	0.7

Table 11. The solutions of the utility function optimization and the interactive approaches

Method	Solution $(x_1, x_2, x_3, y_1, y_2, y_3, y_4)$	*Overal Utility*	***NRD***
Utility function optimization approach	$(0.07, 0.42, -1.25, 126.44, 1436.21, 475.78, 68.21)$	0.792	0.73
Interactive approach (Lee et al. 2011)	$(0.18, 0.39, -1.39, 124.5, 1500, 475.00, 67.50)$	0.786	0.724

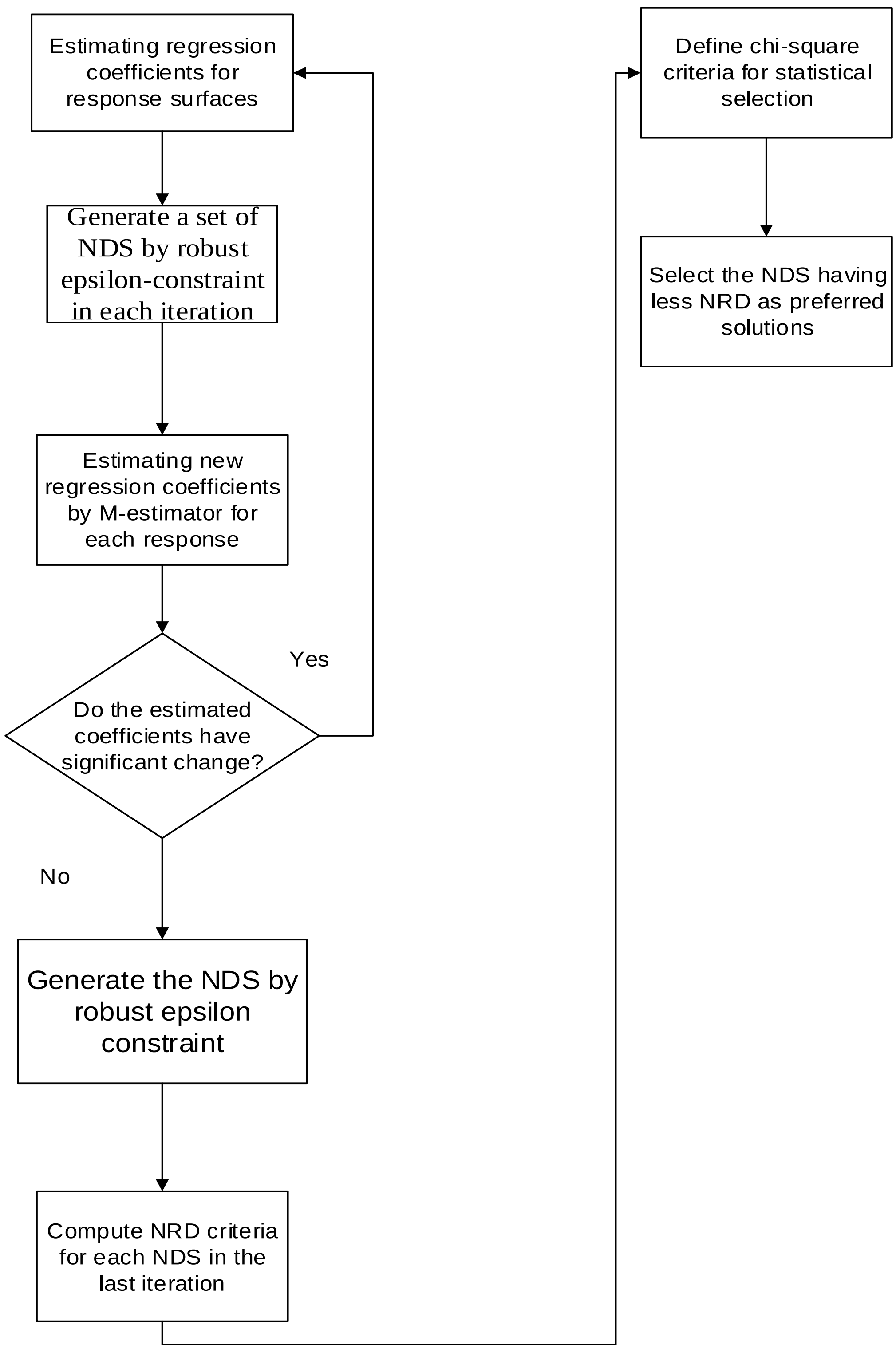

Figure 1. Flowchart of the proposed approach

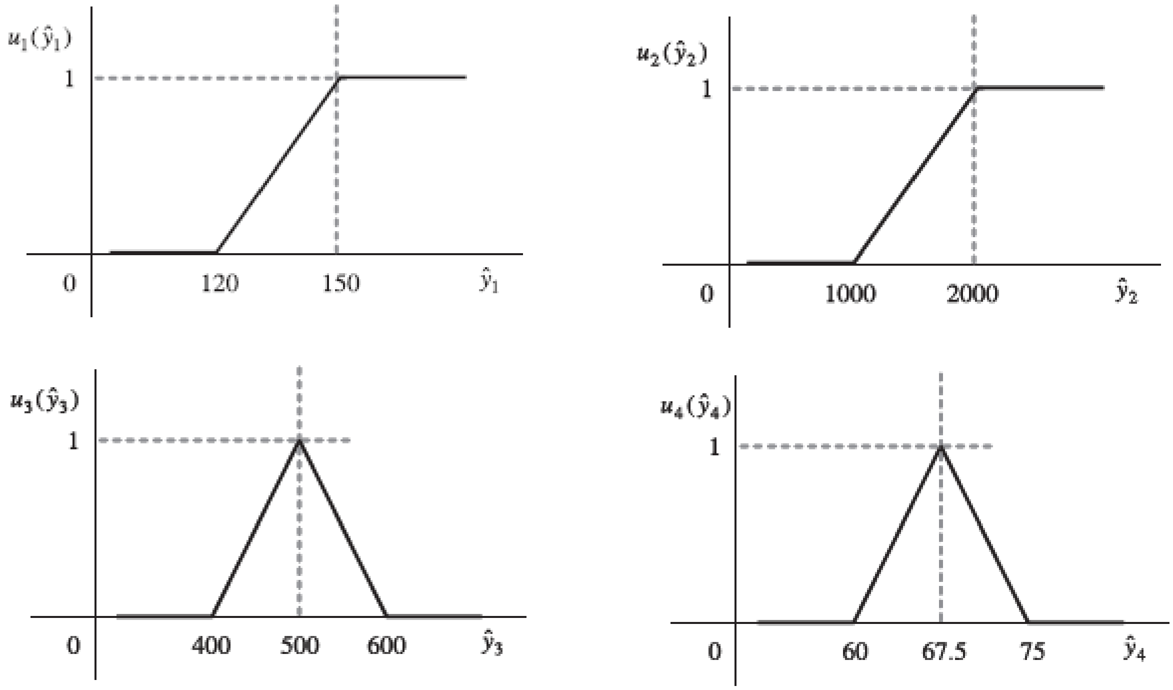

Figure 2. Utility functions of the four responses